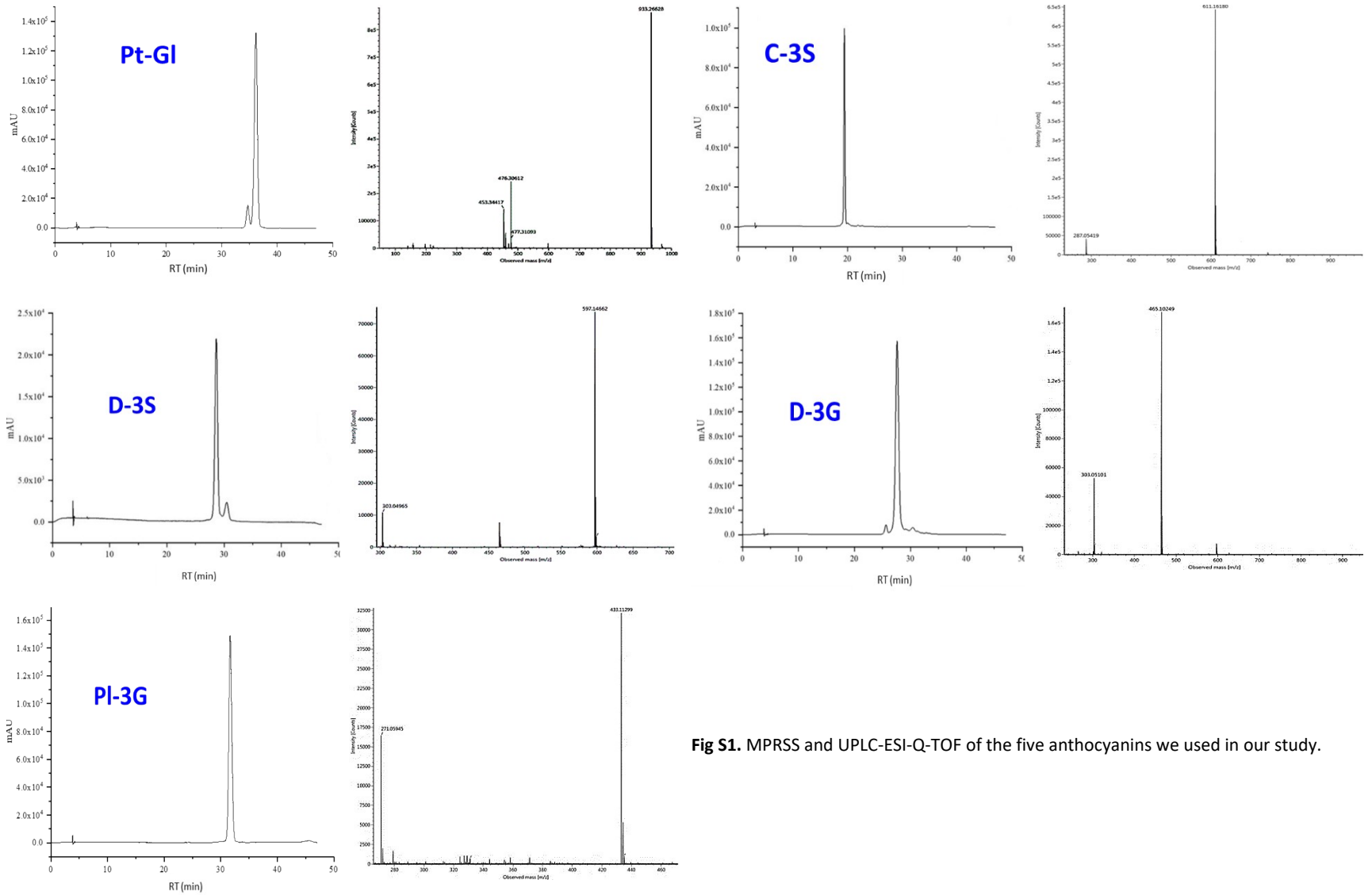
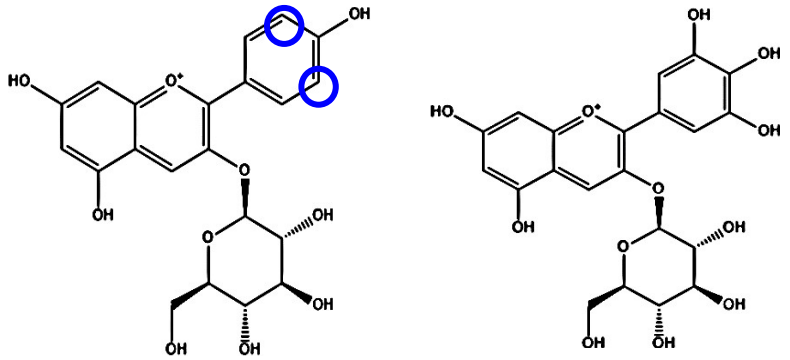
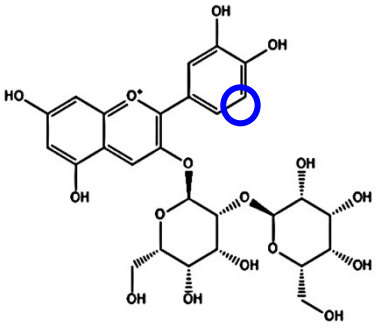


Fig S1. MPRSS and UPLC-ESI-Q-TOF of the five anthocyanins we used in our study.

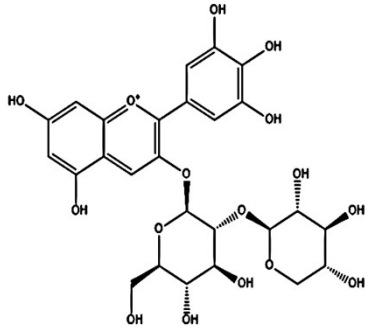


Pl-3G

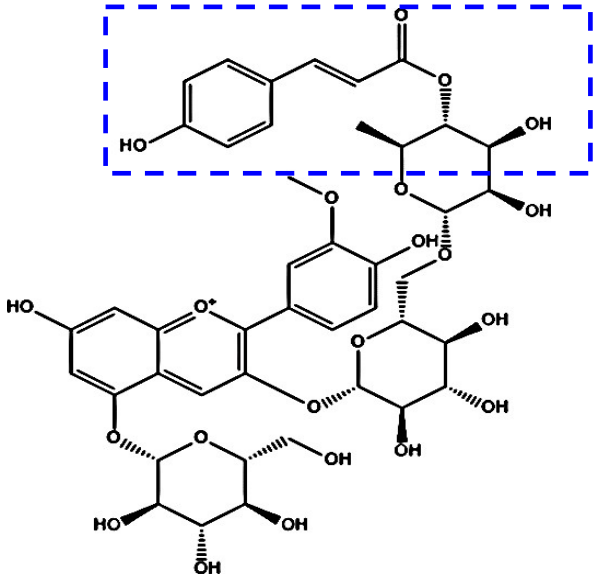
D-3G



C-3S



D-3S



Pt-Gl

Figure S2. The structure for the five anthocyanins. The first row represents the structure for mono-glucoside, the second row represents the structure of di-glycoside, and the third row represent the poly-glycoside anthocyanins.

Table S1. Molecular interaction of different anthocyanins active sties with β-Lg-subunits.

Mixtures	Binding energy (Kcal mol^{-1})	H-bonds	Van der Waals bonds	Hydrophobic bonds	Others	ANs-involved groups
D-3G-β-Lg	5.60	Ser116, Lys69.	--	Pro38, Leu31, Leu39, Ala118, Asn109, Leu117, Glu108, Lys91, Ile56, Asn90.	Pi-Anion: Met107. Pi-Alkyl: Val41, Lys60, Ile71, Val92, Ile84.	C4'-OH-B ring, C and B rings, and glycosyl units.
C-3S-β-Lg	5.22	Lys69, Pro38, Asn90.	--	Leu31, Ser116, Leu117, Ala118, Glu108, Asn109, Ile84, Asp85, Ala86, Asn88, Leu87, Val41, Ile71, Leu58, Lys60.	Pi-Pi Stacked: Met107, Leu39, Pro38.	A, C, and B-rings, and glycosyl units.
Pl-3G-β-Lg	2.55	Ser116, Lys69.	Glu108	Leu31, Leu39, Asn109, Ala118, Leu117, Glu108, Lys91, Ile56, Leu58, Pro8.	Pi-Anion: Met107. Pi-Alkyl: Val41, Lys60, Ile71, Val92, Ile84, Met107	C4'-OH-B ring, C and B rings, and glycosyl units.
D-3S-β-Lg	3.24	Lys69, Asp85, Ala118.	Lys60, Asn88.	Ala86, Leu87, Asn109, Ser116, Leu117, Leu31, Glu108, Lys91, Leu39, Asn90, Pro38, Leu58, Ile56.	Pi-Anion: Met107. Pi-Alkyl: Val41, Ile71, Met107, Val92, Ile84.	C7-OH-A ring, C6-H- A ring, C and B rings, and glycosyl units.
Pt-Gl-β-Lg	1.58	His161, Tyr20, Glu127, Thr125, Lys101, Arg124.	--	Val123, Asp129, Val128, Leu166, Cys160, Glu158, Gln159, Gln59, Tyr42, Val43, Thr18, Glu157, Pro126, Trp19, Val43, Ser21.	Pi-Anion: Glu44. Pi-Alkyl: Lys100. Pi-Pi Stacked: Tyr20.	B-ring, glycosyl units, and acylated part.

Table S2. Partition coefficient for octanol water mixture (ClogP), molecular weight, number of H-bonds donor or acceptor, volume, and polar surface area for the five different anthocyanins (SYBYL-X 2.0).

Anthocyanins	CLogP	Molecular weight	Donor count	Acceptor count	Volume	Polar surface area
Pl-3G	-1.75	433.39	7	10	1050.80	313.07
D-3G	-3.01	465.38	9	12	1101.04	382.34
D-3S	-4.50	597.50	11	16	1330.81	399.58
C-3S	-3.87	611.53	11	16	1360.64	445.19
Pt-Gl	-2.66	917.84	12	22	2241.70	505.43